

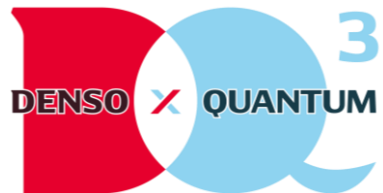


# Partition of Large Optimization Problems with One-Hot Constraint

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# Take-home messages

Motivation:

Solving large optimization problems with the one-hot constraint efficiently.

Message1:

For difficult optimization problems with frustrations, the proposed methods are effective in improving solutions.

Message2:

One of the proposed methods releases us from adjusting  $\lambda$ , which controls the strength of the one-hot constraint.

# Agenda

1. Optimization of large problems using D-Wave
2. Proposed methods
3. Assessment of solution accuracy
4. Discussion on the results
5. Summary

# 1.

## Optimization of large problems using D-Wave

# Limitations of the current D-Wave machine

## ■ Ising model of D-Wave machine

### ① Number of qubits

$$\mathcal{H} = \sum_{(i,j) \in \text{Chimera}}^{N_q} J_{ij} \sigma_i \sigma_j + \sum_{i=1}^{N_q} h_i \sigma_i$$

### ② Restricted to Chimera graph

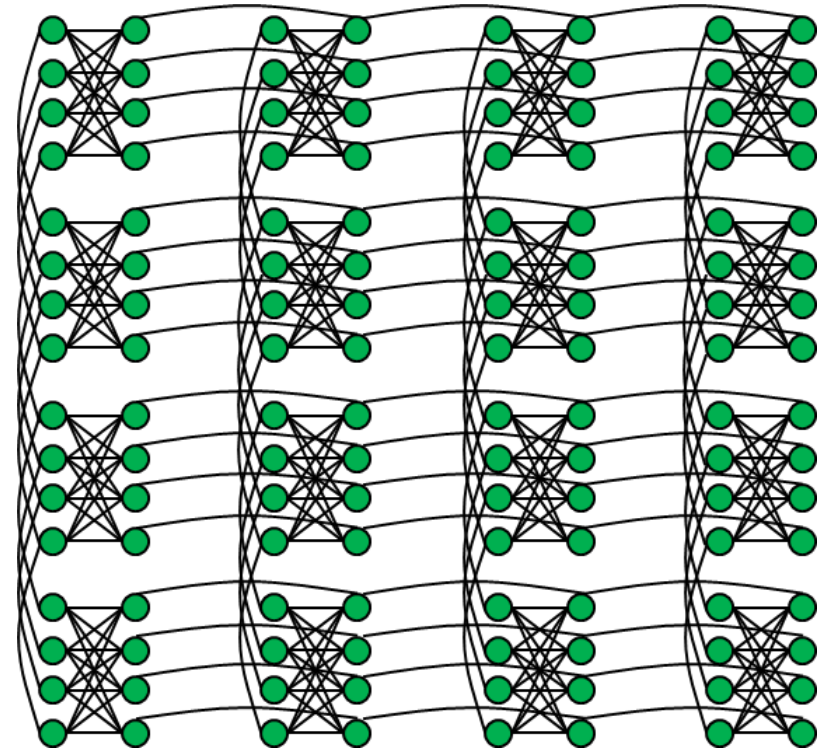
## ■ Practical optimization problem

### ① Large number of variables

$$\mathcal{H} = \sum_{i < j}^{N_p} J_{ij} x_i x_j + \sum_{i=1}^{N_p} h_i x_i$$

### ② Between arbitrary variables

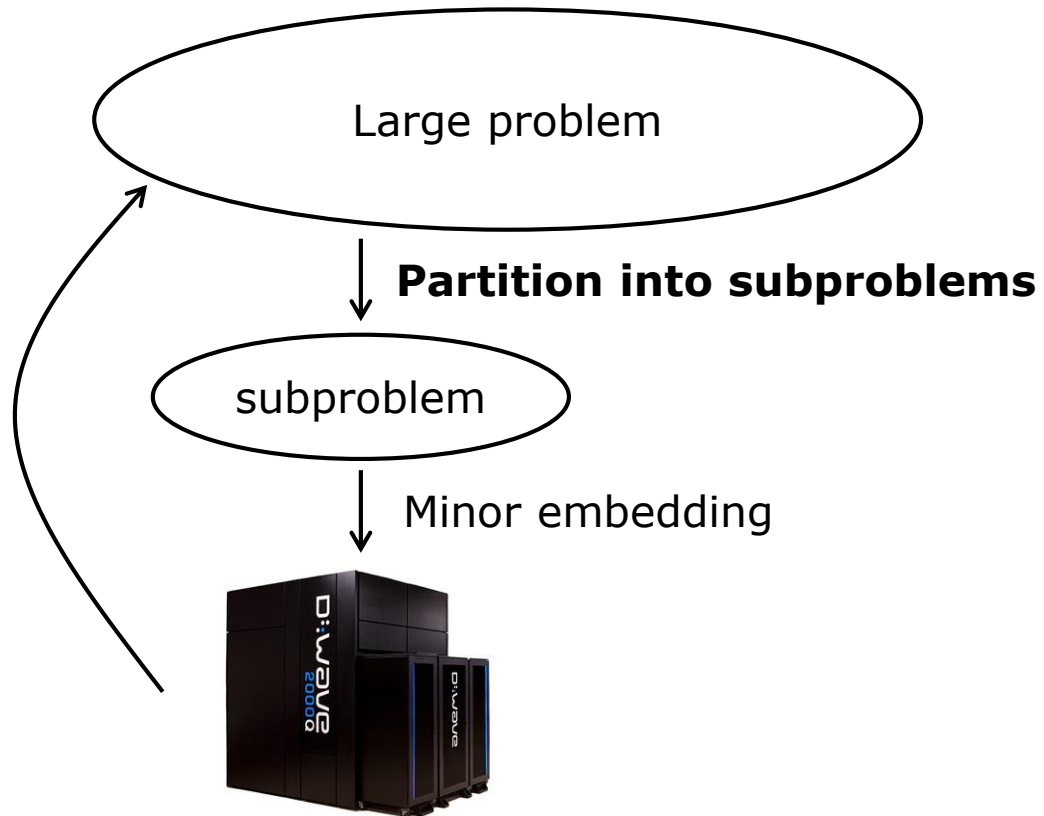
## ■ Structure of Chimera graph



**Partitioning and embedding are required to solve practical optimization problems.  
In this talk, we focus on the partition of large optimization problems.**

# Conventional tool: qbsolv

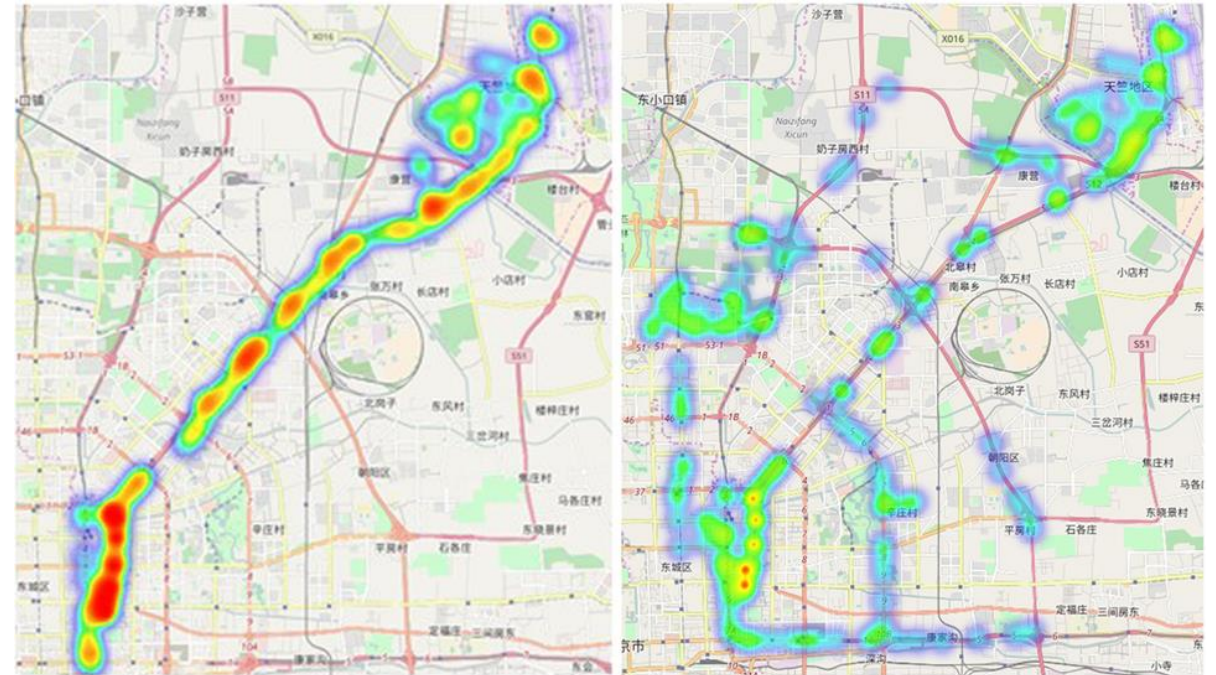
## ■ Optimization process of qbsolv



We propose efficient partitioning of large problems with the one-hot constraint.

**We propose efficient partitions for the problems with one-hot constraint.**

## ■ Example of a problem with one-hot constraint < Traffic flow optimization by VW >



F. Neukart, et. al., Front. ICT **4**, 29 (2017)

Select one route from three options for each taxi to minimize traffic congestion

# 2.

## Proposed methods

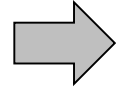
# One-hot representation

<Original cost function>

$$\mathcal{H}_0 = \sum_{i < j} J_{ij} \delta(S_i, S_j)$$

$$S_i \in (1, 2, \dots, Q)$$

variable with Q components

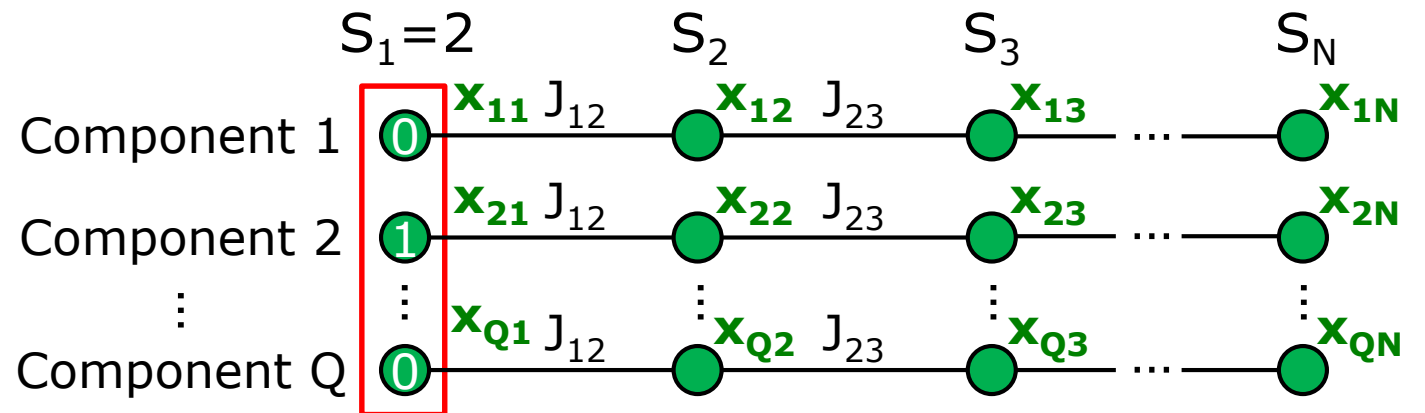


<Cost function with one-hot constraint>

$$\mathcal{H}_0 = \sum_{i < j} J_{ij} \sum_{q=1}^Q x_{qi} x_{qj} + \lambda \sum_{i=1}^N \left( \sum_{q=1}^Q x_{qi} - 1 \right)^2$$

one-hot constraint

$$x_{qi} \in (0, 1)$$



Only Q of  $2^Q$  states satisfy the one-hot constraint for each  $S_i$ .

**A fraction of states satisfy the one-hot constraint.**

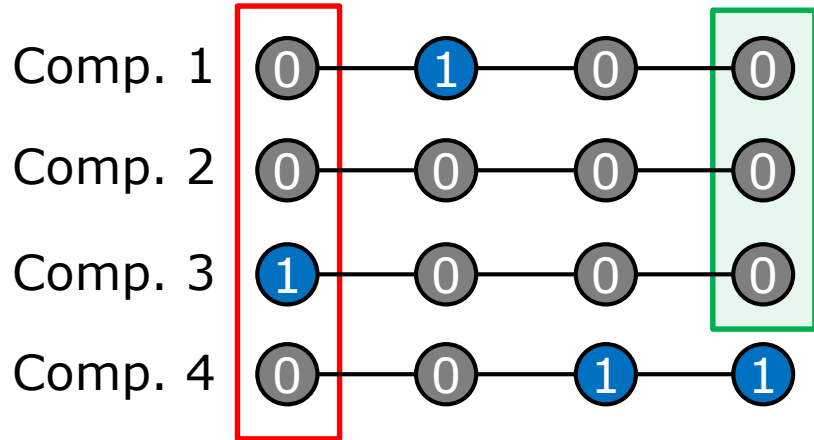


# Simple example of bad partition

We should pay attention whether states satisfying the constraint are included or not.

< Current solution >

$S_1=3$   $S_2=1$   $S_3=4$   $S_4=4$

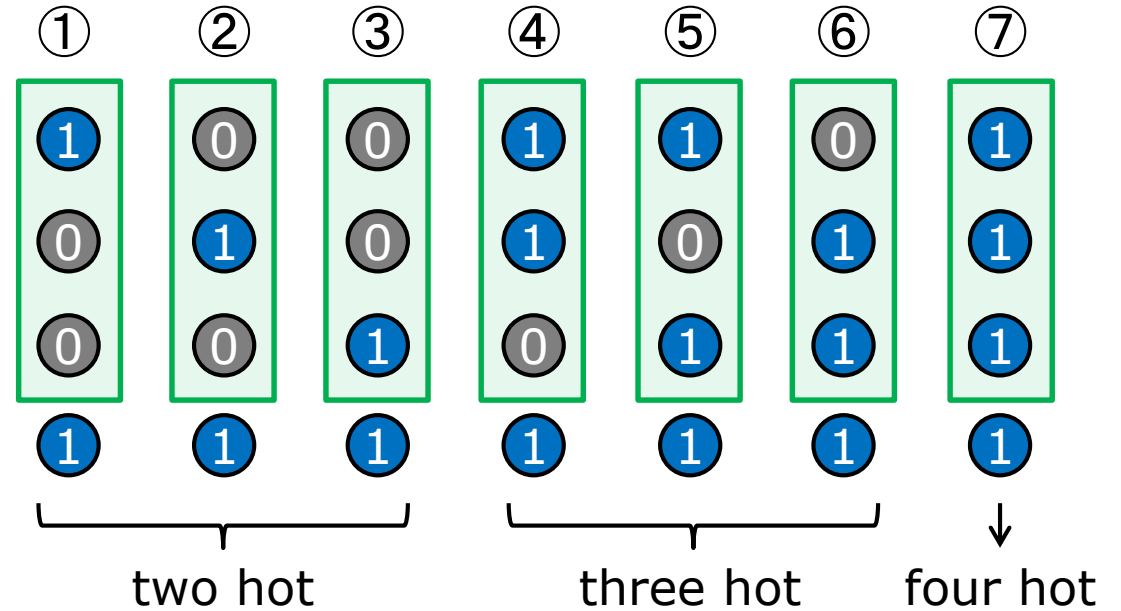


one-hot constraint

①: currently selected component

Extract as a subproblem

< Candidates of transition destinations >



No destinations satisfy the one-hot constraint.

**Better solutions cannot be searched by the optimization of the subproblem.**

# Proposed methods

Two methods to extract subproblems including states that satisfy the constraint.

	Multivalued partition	Binary partition
Summary	<p>Extract subproblems that contain current comp. for each variable</p> <p>subproblem (more than two components) ①: currently selected component</p>	<p>Extract a binary subproblem.</p> <p>Select exactly one component in addition to the current comp.</p> <p>subproblem with two components ①: currently selected component</p> <p>Make binary subproblem; "stay or transit" binary variable: <math>\{y_i\}</math></p> <p>embed subproblem</p>
Pros	<ul style="list-style-type: none"> <li>Destinations satisfying the one-hot constraint exist for all variables.</li> </ul>	<ul style="list-style-type: none"> <li>All states satisfy the constraint, and <math>\lambda</math> disappears.</li> <li>Large number of variables can be embedded.</li> </ul>
Cons	<ul style="list-style-type: none"> <li>Not all states satisfy the constraint.</li> </ul>	<ul style="list-style-type: none"> <li>Only two components are considered at one time.</li> </ul>

# 3.

## Assessment of solution accuracy

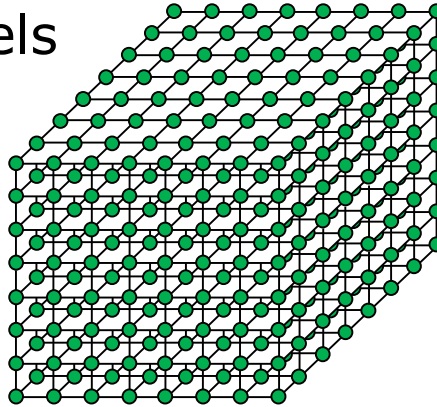
# Problem settings 1/2

## ■ Cost function

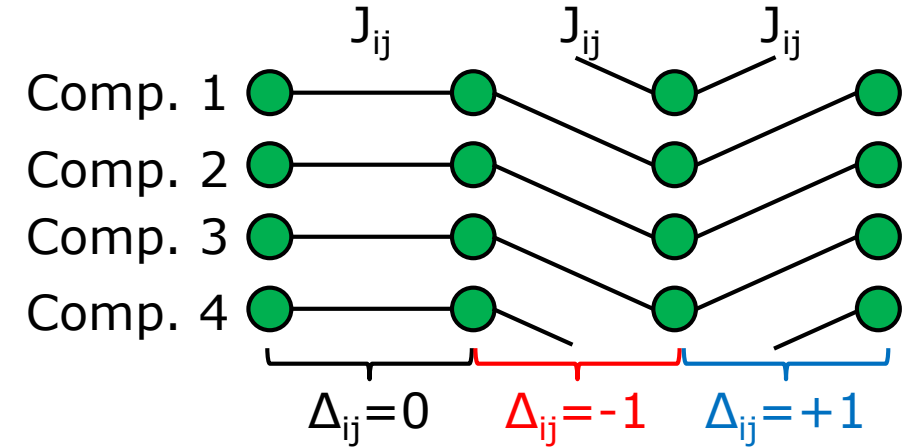
3D-4 components Potts models with 10x10x10 variables

$$\mathcal{H}_0 = - \sum_{\langle ij \rangle} J_{ij} \delta_{S_i, S_j + \Delta_{ij}}$$

$$S_i \in (1, 2, 3, 4)$$



## ■ Problem graph



## ■ Parameters

model	$J_{ij}$	$\Delta_{ij}$
Ferromagnetic model	-1	0
Anti-ferromagnetic model	+1	0
Potts glass model	+1(50%) or -1(50%)	0
Potts gauge glass model	-1	0(50%) or +1(25%) or -1(25%)

**Easy problem**

**Hard problem**

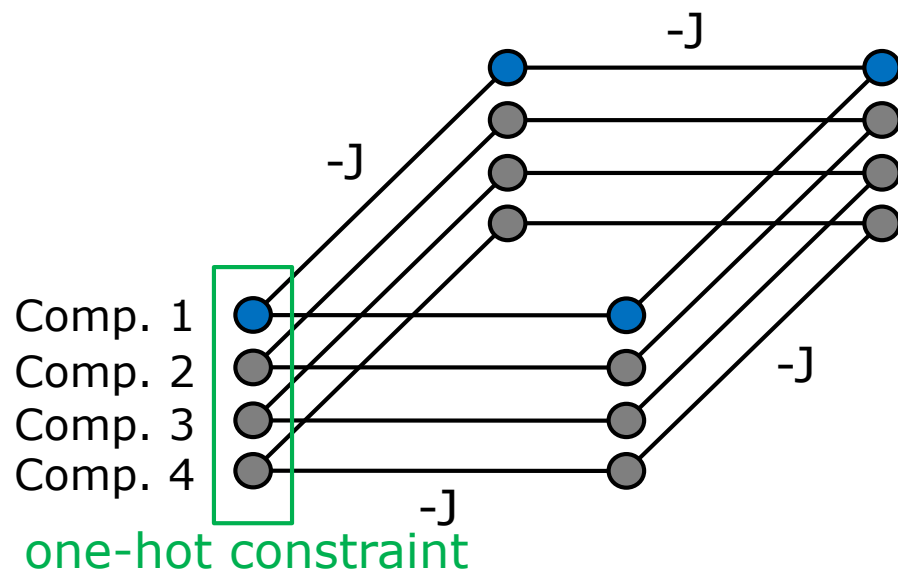
**We evaluate solution accuracy for the several Potts models.**

# Problem settings 2/2

Simple examples of a ground state of the Potts models.

## ■ Ferromagnetic Potts model

Interactions between same components exist.

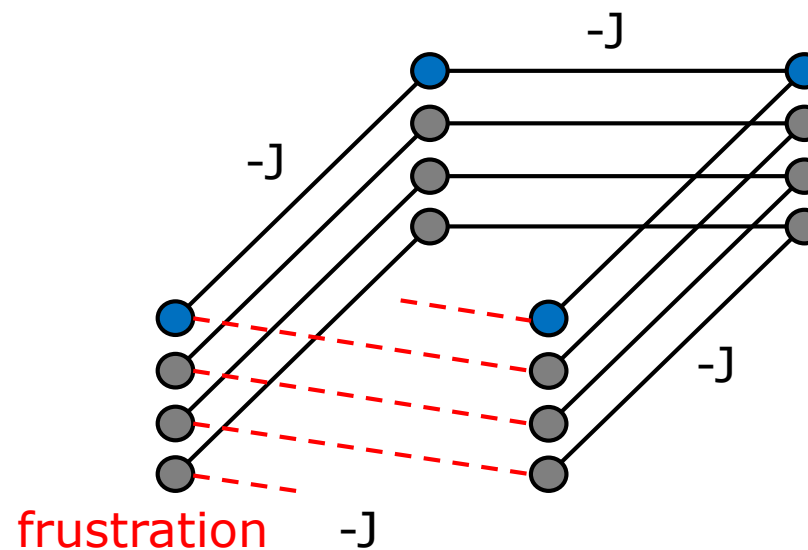


● :selected component

All interactions can be satisfied;  
trivial ground state

## ■ Potts gauge glass model

Interactions between different components exist.

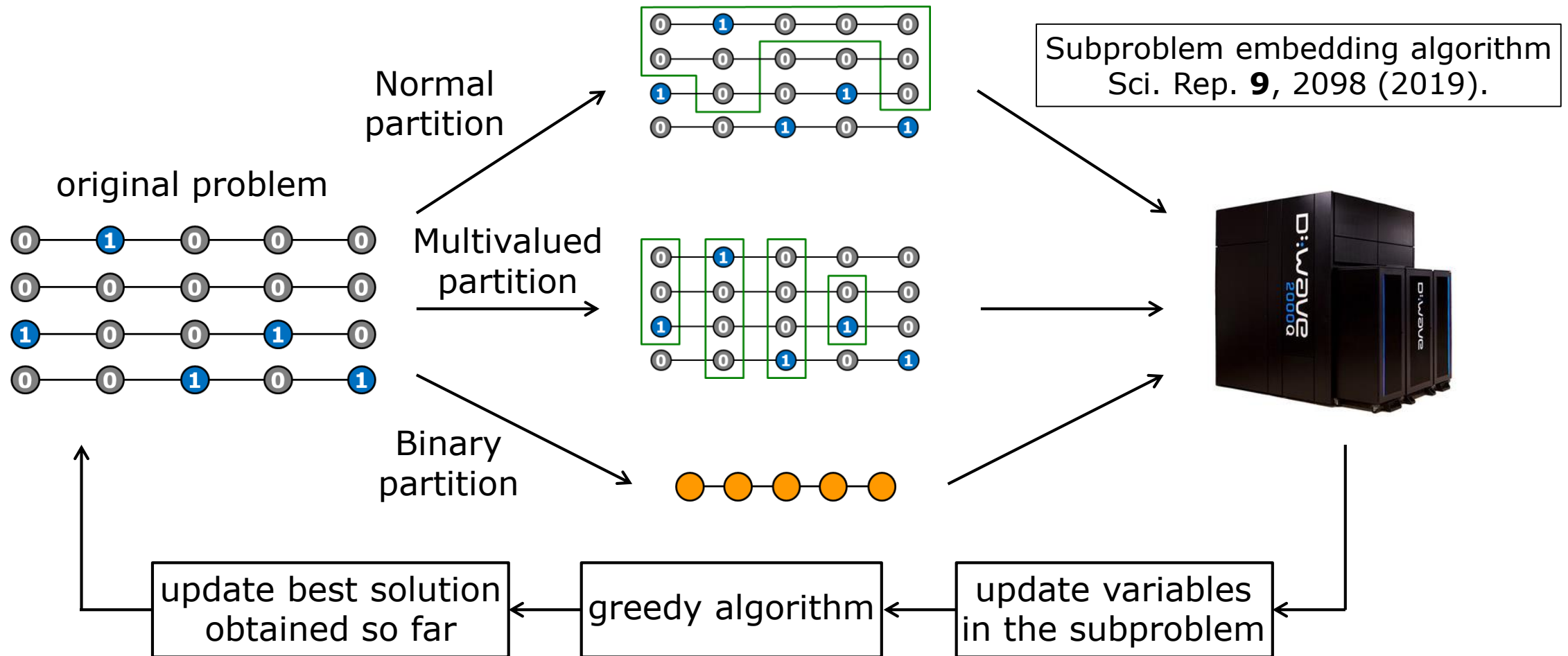


● :selected component

All interactions cannot be satisfied;  
non-trivial ground state

**The ground states of the hard problem is non-trivial.**

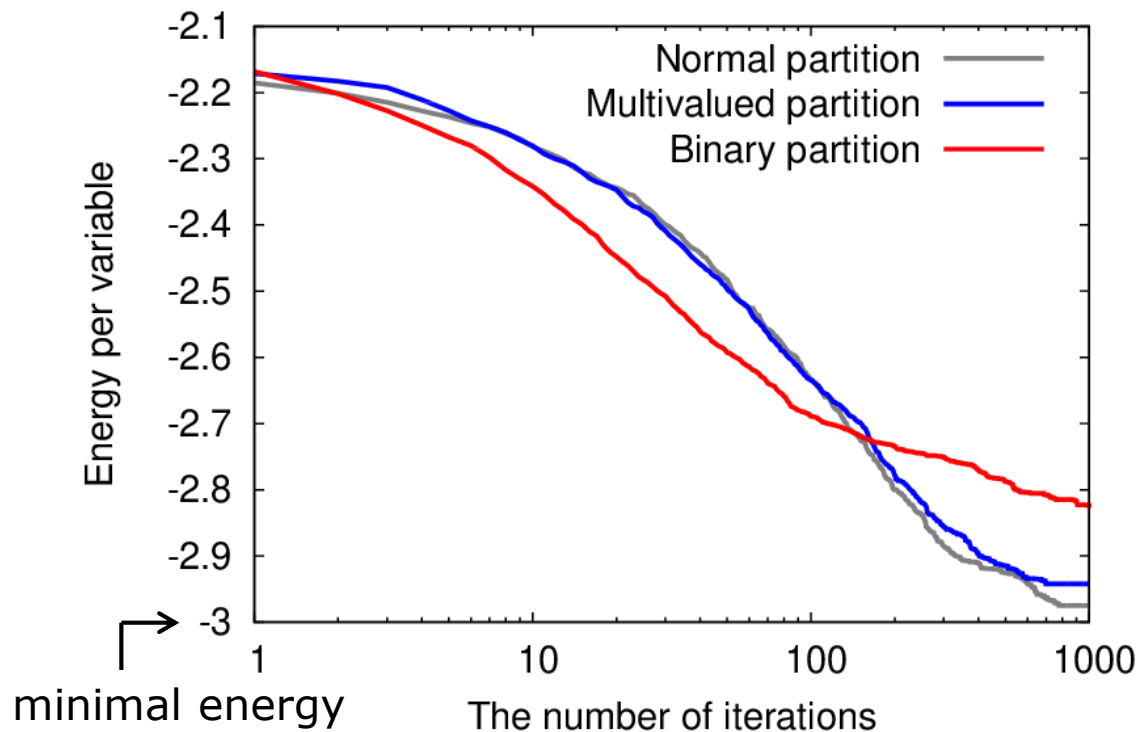
# Optimization process



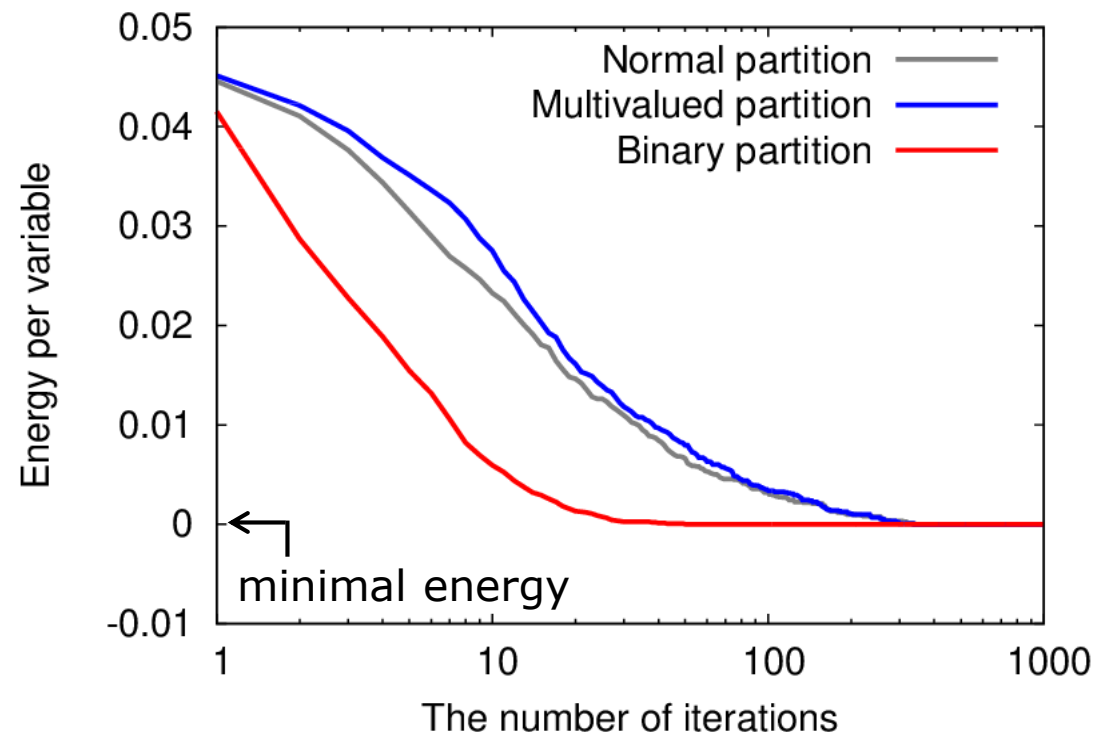
**We compare solution accuracy for three partitioning methods.**

# Results for the easy problems

<Ferromagnetic model>



<Anti-ferromagnetic model>

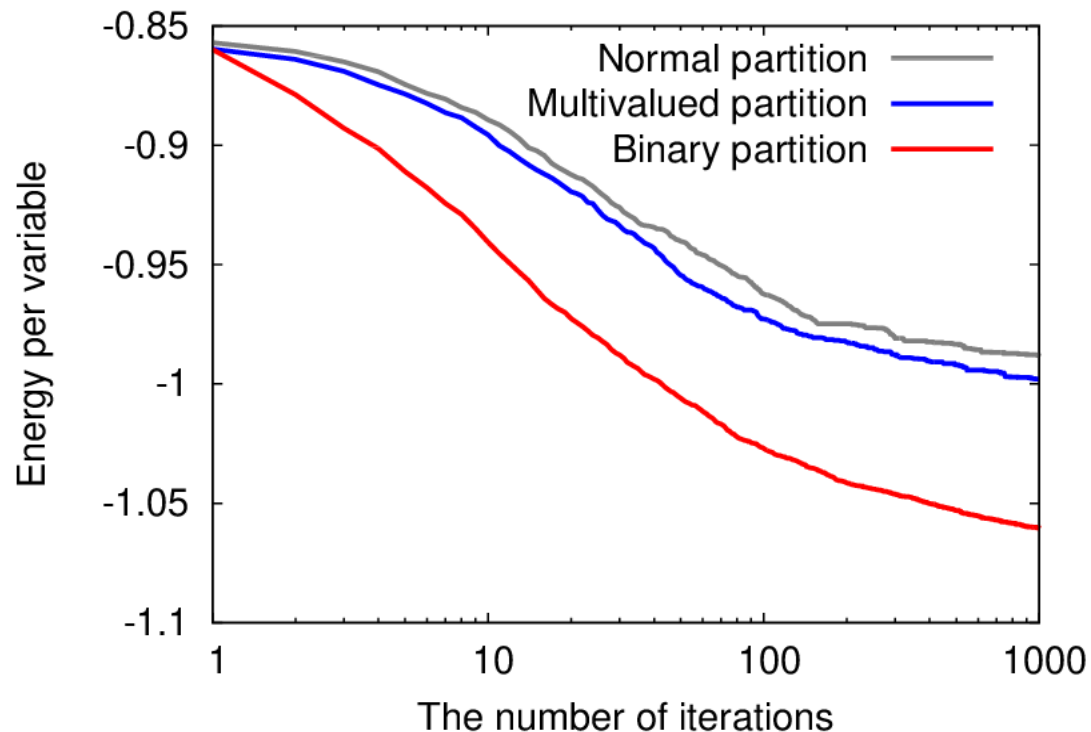


**Performance of normal and multivalued partitions are almost same.**

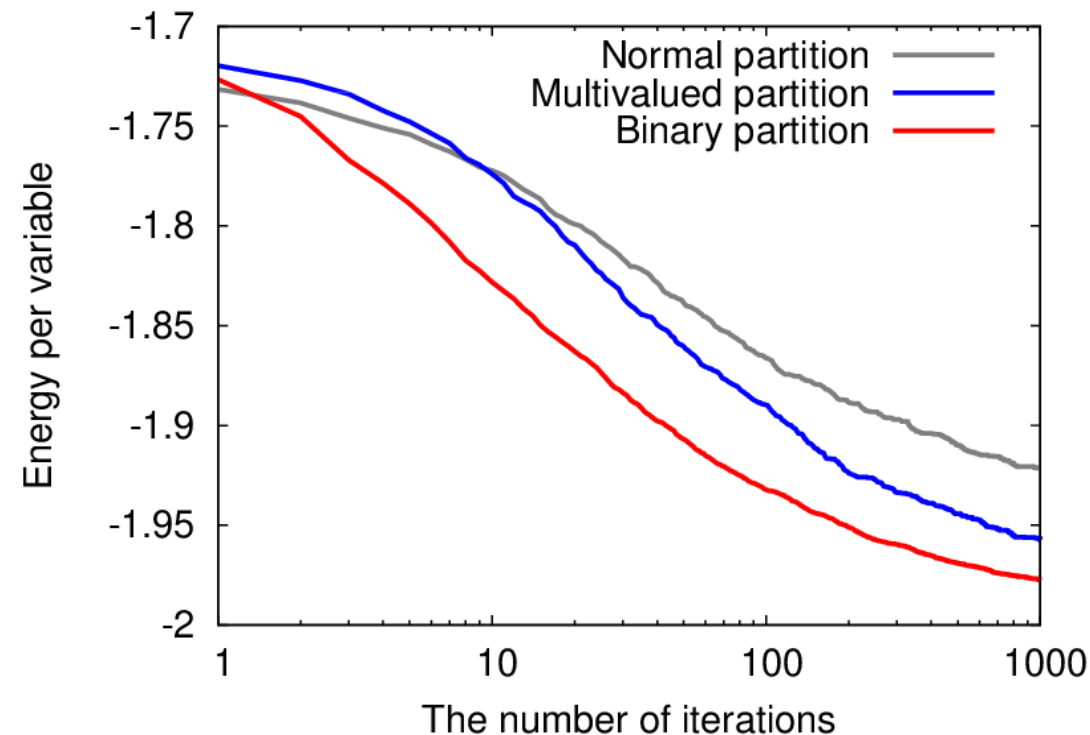
**The energy obtained by binary partition differs from that of others.**

# Results for the hard problems

<Potts glass model>



<Potts gauge glass model>



**Performance of multivalued partition is better than that of normal one.  
The binary partition shows the best performance for the hard problems.**

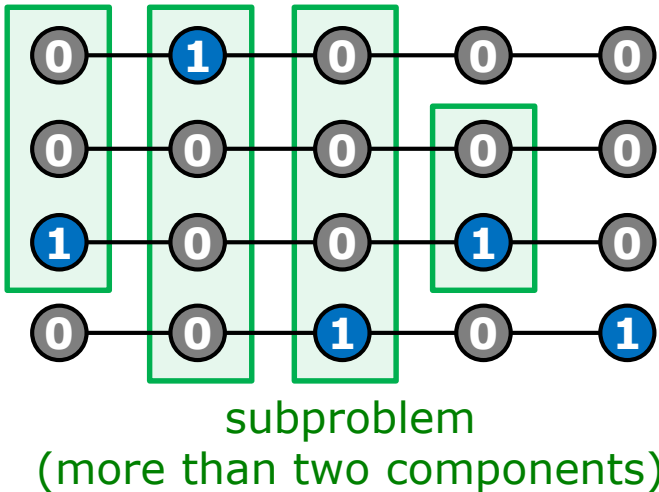
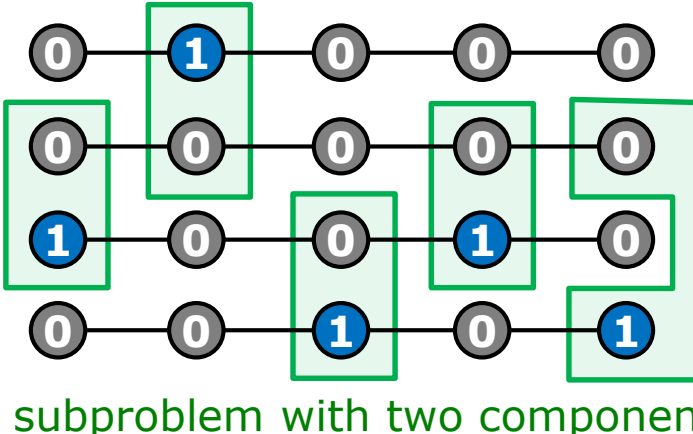
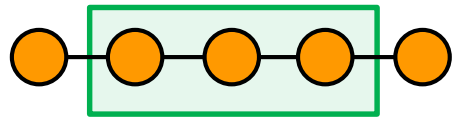



# 4.

## Discussion on the results

# Proposed methods

Two methods to extract subproblems including states that satisfy the constraint.

	Multivalued partition	Binary partition
Summary	<p>Extract subproblems that contain current solution for each variable</p>  <p>subproblem (more than two components)</p> <p>① : current solution</p>	<p>Extract a binary subproblem.</p> <p>Randomly select two comps. in addition to current solutions</p>  <p>subproblem with two components</p> <p>① : current solution</p> <p>Extract binary subproblem; "transit or not"</p> <p>binary variable: <math>\{y_i\}</math></p>  <p>embed subproblem</p> 
Pros	<ul style="list-style-type: none"> <li>Destinations satisfying the one-hot constraint exist for all variables.</li> </ul>	<ul style="list-style-type: none"> <li>All states satisfy the constraint, and <math>\lambda</math> disappears.</li> <li>Large number of variables can be embedded.</li> </ul>
Cons	<ul style="list-style-type: none"> <li>Not all states satisfy the constraint.</li> </ul>	<ul style="list-style-type: none"> <li><b>Only two components are considered at one time.</b></li> </ul>

# Discussion: Binary partition for the ferromagnetic model

## ■ Question

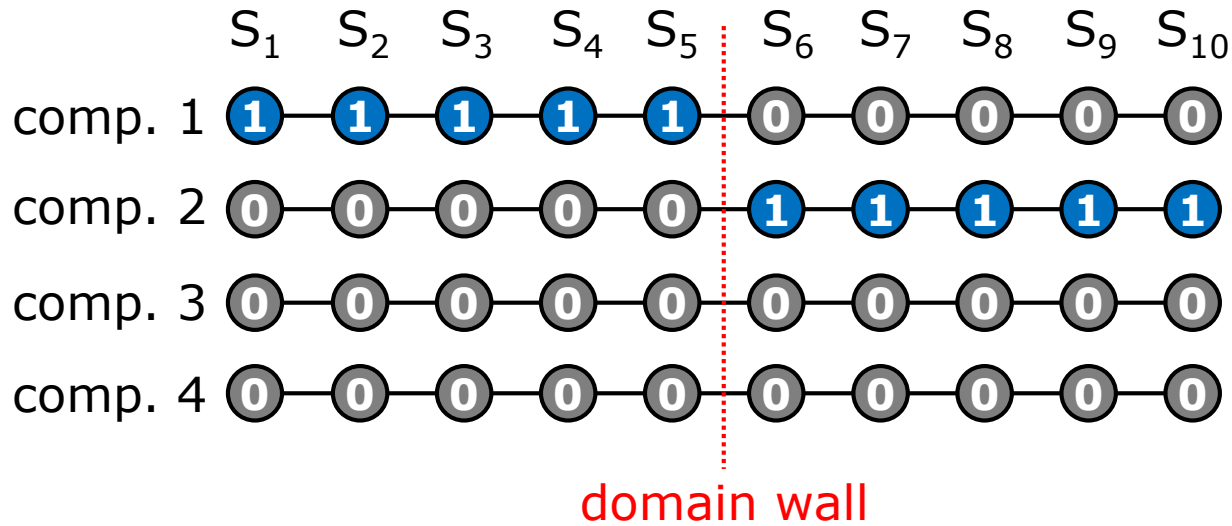
Why is the performance of the binary partition remarkably bad for the ferromagnetic model?

## ■ Answer

Subproblems which can eliminate domain walls are rarely extracted.

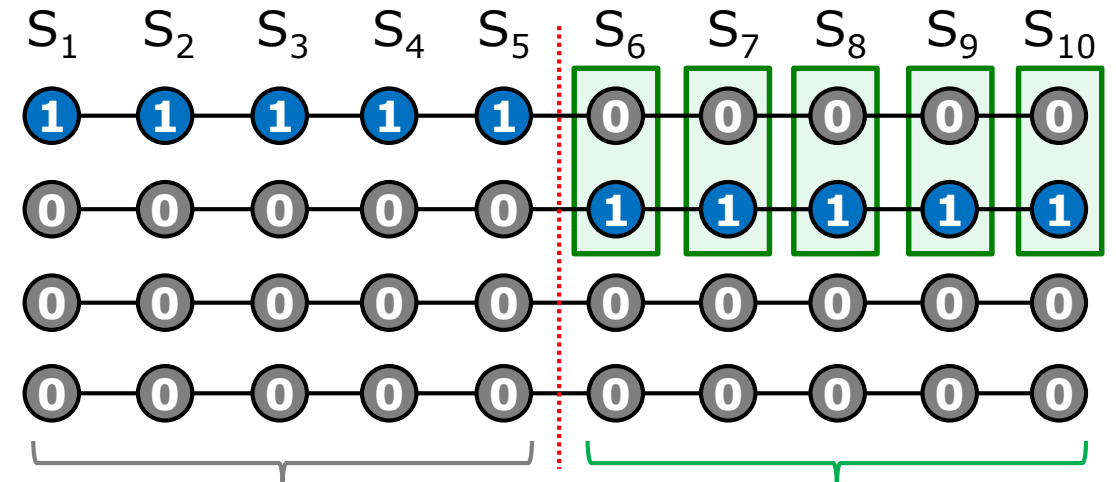
<Current solution>

1D ferromagnetic Potts model with ten variables



One of the first excited states which often appear.

<Subproblem to align all variables to comp. 1>



any component

Comp. 1 must be included;  
probability =  $(1/3)^5 = 1/243$

## The binary partition is not suitable for the ferromagnetic model.

# Discussion: Binary partition for the anti-ferromagnetic model

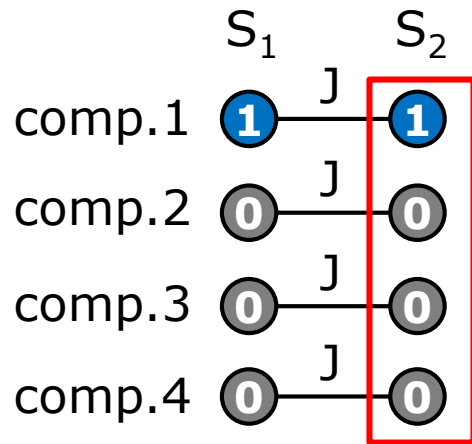
## ■ Question

Why is the performance of the binary partition remarkably high for the anti-ferromagnetic model?

## ■ Answer

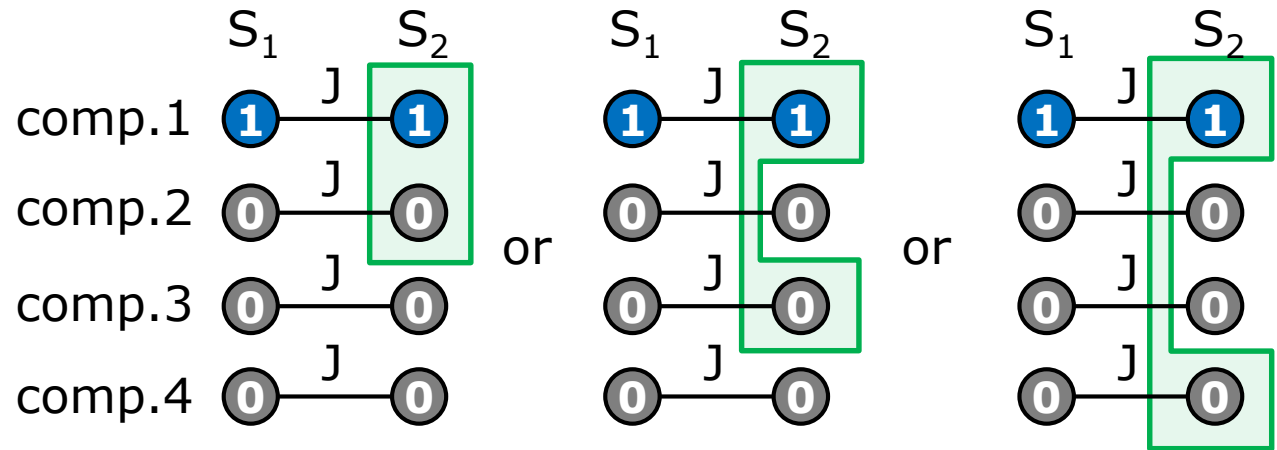
There exist many binary subproblems that reduce the energy.

<Current solution>



Suppose that we update the variable  $S_2$ .  
 $S_2 \neq 1$  reduce the energy.

<Binary subproblems to improve the current solution>



All binary subproblems can improve the current solution.  
 $\Rightarrow$  Extracting only two components is sufficient.

**The existence of many low-energy transition destinations is essential.**

# Discussion: Binary partition for the hard problems

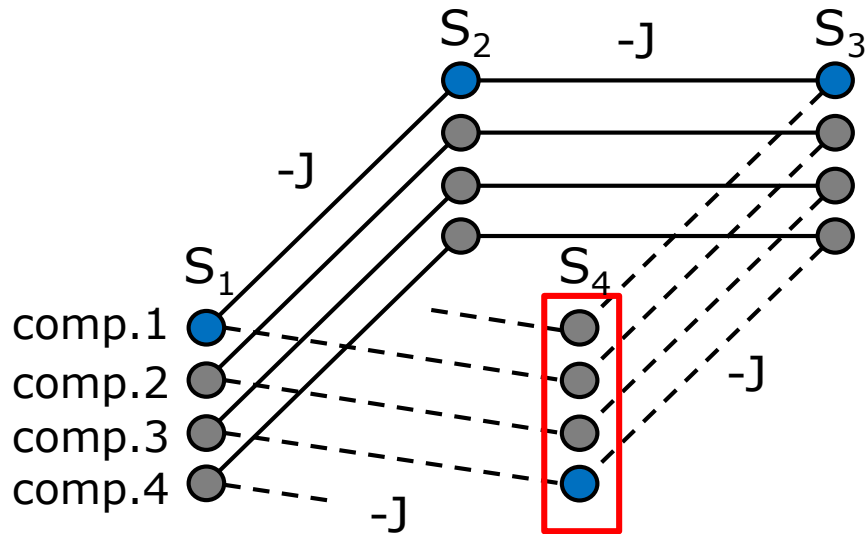
## ■ Question

Why is the performance of the binary partition high for the hard problems?

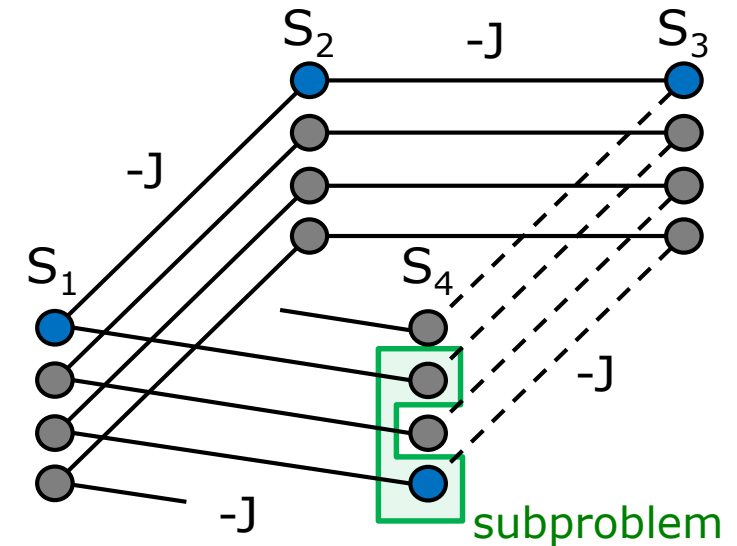
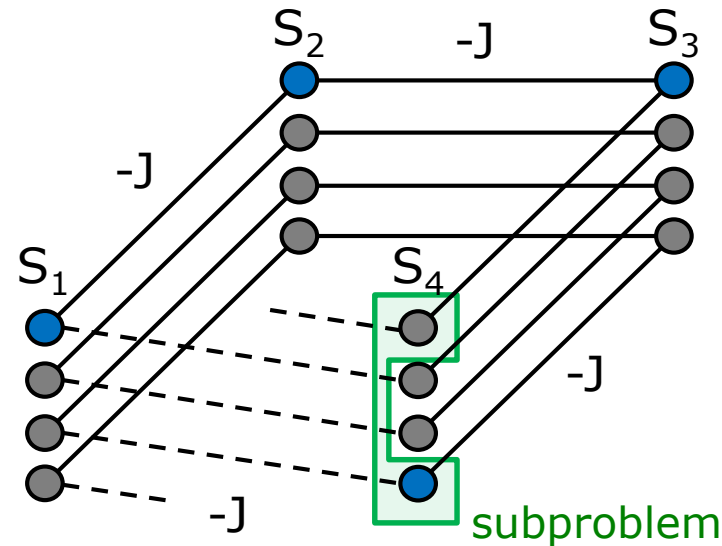
## ■ Answer

There exist many low-energy destinations caused by frustrations.

< Current solution >



< Binary subproblems to improve the current solution >



Suppose that we update the variable  $S_4$ .  
Ground states satisfy three interactions.

There are two states that satisfy three interactions  
⇒ Two of three binary subproblems can reduce the energy.

**The binary partition is suitable for the problems with frustrations.**

# Summary of this talk

## ■ Summary

- We proposed two partitioning methods for problems with the one-hot constraint.
- The binary partition shows best performance except for the ferromagnetic model.
- The binary partition is suitable for problems with many low-energy destinations.
- The binary partition contains only constraint-satisfying states, and we do not need to adjust the parameter  $\lambda$ .
- We could not find problems for which the multivalued partition is suitable.

## ■ Future work

- Construct new algorithms to efficiently optimize the ferromagnetic model using the binary partition.

***DENSO***

Crafting the Core

# Discussion: Normal partition for the easy problems

## ■ Question

Why is the performance of the multivalued partition is not superior to the normal one?

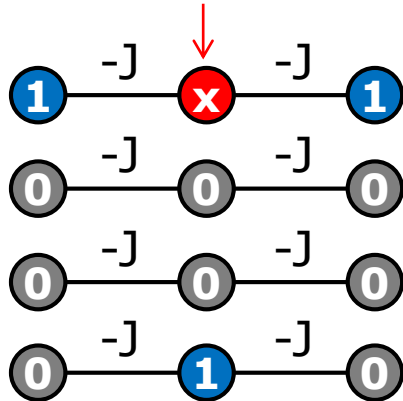
## ■ Answer

Transitions that violate the one-hot constraint can reduce the energy for the easy problems.

<Simple example of normal partition>

1D ferromagnetic Potts model

extract one-variable subproblem



<Energy of the subproblem>

$$E(x = 1) = \underbrace{-2J}_{\text{interaction}} + \underbrace{\lambda}_{\text{constraint (penalty)}}$$

$$E(x = 0) = 0$$

If  $\lambda$  is not so large ( $\lambda < 2J$ )

transitions violating the constraint can reduce the energy.

**Multivalued partition is not so effective in improving solutions, if there exist states that satisfy many interactions simultaneously.**